# A Model-Based Frequency Constraint for Mining Associations from Transaction Data

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**Abstract**

Mining frequent itemsets is a popular method for finding associated items in databases. For this method, support, the co-occurrence frequency of the items which form an association, is used as the primary indicator of the associations's significance. A single user-specified support threshold is used to decided if associations should be further investigated. Support has some known problems with rare items, favors shorter itemsets and sometimes produces misleading associations.

In this paper we develop a novel model-based frequency constraint as an alternative to a single, user-specified minimum support. The constraint utilizes knowledge of the process generating transaction data by applying a simple stochastic mixture model (the NB model) which allows for transaction data's typically highly skewed item frequency distribution. A user-specified precision threshold is used together with the model to find local frequency thresholds for groups of itemsets. Based on the constraint we develop the notion of NB-frequent itemsets and adapt a mining algorithm to find all NB-frequent itemsets in a database. In experiments with publicly available transaction databases we show that the new constraint provides improvements over a single minimum support threshold and that the precision threshold is more robust and easier to set and interpret by the user.

**Keywords:** Data mining, associations, interest measures, mixture models, transaction data.

## 1 Introduction

Mining associations (i.e., set of associated items) in large databases has been under intense research since Agrawal et al. (1993) presented *Apriori*, the first algorithm using the support-confidence framework to mine frequent itemsets and association rules. The enormous interest in associations between items is due to their direct applicability for many practical purposes. Beginning with discovering regularities in transaction data recorded by point-of-sale systems to improve sales, associations are also used to analyze Web usage patterns (Srivastava et al., 2000), for intrusion detection (Luo and Bridges, 2000), for mining genome data (Creighton and Hanash, 2003), and for many other applications.

An association is a set of items found in a database which provides useful and actionable insights into the structure of the data. For most current applications support is used to find potentially useful associations. Support is a measure of significance defined as the relative frequency of an association in the database. The main advantages of using support are that it is simple to calculate, no assumptions about the structure of mined data are required, and support possesses the a so-called *downward closure property* (Agrawal and Srikant, 1994) which makes a more efficient search for all frequent itemsets in a database possible. However, support has also some important shortcomings. Some examples found in the literature are:

- Silverstein et al. (1998) argue with the help of examples that the definition of association rules (using support and confidence) can produce misleading associations. The authors suggest using statistical tests instead of support to find reliable dependencies between items.

- Support is prone to the rare item problem (Liu et al., 1999) where associations including items with low support are discarded although they might contain valuable information.
- Support favors smaller itemsets while longer itemsets could still be interesting, even if they are less frequent (Seno and Karypis, 2001). In order to find longer itemset, one would have to lower the support threshold which would lead to an explosion of the number of short itemsets found.

Statistics provides a multitude of models which proved to be extremely helpful to describe data frequently mined for associations (e.g., accident data, market research data including market baskets, data from medical and military applications, and biometrical data (Johnson et al., 1993)). For transaction data, many models build on mixtures of counting processes which are known to result in extremely skewed item frequency distributions with very few relatively frequent items while most items are infrequent. This is especially problematic since support's rare item problem affects the majority of items in such a database. Although the effects of skewed item frequency distributions in transaction data are sometimes discussed (e.g. by Liu et al. (1999) or Xiong et al. (2003)), most current approaches neglect knowledge about statistical properties of the generating processes which underlie the mined databases.

The contribution of this paper is that we address the shortcomings of a single, user-specified minimum support threshold by departing from finding frequent itemsets. Instead we propose a model-based frequency constraint to find NB-frequent itemsets. For this constraint we utilizes knowledge of the process which underlies transaction data by applying a simple stochastic baseline model (an extension of the NB model) which is known for its wide applicability. A user-specified precision threshold is used to identify local frequency thresholds for groups of associations based on evaluating observed deviations from a baseline model. The proposed model-based constraint has the following properties:

1. It reduces the problem with rare items since the used stochastic model allows for highly skewed frequency distributions.
2. It is able to produce longer associations without generating an enormous number of shorter, spurious associations since the support required by the model is set locally and decreases with the number of items forming an association.
3. Its precision threshold parameter can be interpreted as a predicted error rate. This makes communicating and setting the parameter easier for domain experts. Also, the parameter seems to be less dependent on the structure of the database than support.

The rest of the paper is organized as follows: In the next section we review the background of mining associations and some proposed alternative frequency constraints. In Section 3 we develop the model-based frequency constraint, the concept of NB-frequent itemsets, and show that the chosen model is useful to describe real-word transaction data. In Section 4 we present an algorithm to mine all NB-frequent itemsets in a database. In Section 5 we investigate and discuss the behavior of the model-based constraint using several real-world and artificial transaction data sets.

# 2 Background and Related Work

The problem of mining associated items (frequent itemsets) from transaction data was formally introduced by Agrawal et al. (1993) for mining association rules as: Let $I = \{i_1, i_2, ..., i_n\}$ be a set of $n$ distinct literals called items and $\mathcal{D} = \{t_1, t_2, ..., t_m\}$ a set of transactions called the database. Each transaction in $\mathcal{D}$ contains a subset of the items in $I$. A rule is defined as an implication of the from $X \longrightarrow Y$ where $X, Y \subseteq I$ and $X \cap Y = \emptyset$. The sets of items (for short itemsets) $X$ and $Y$ are called antecedent and consequent of the rule. An itemset which contains $k$ items is said to

have length or size $k$ and is called a $k$-itemset. An itemset which is produced by adding a single item to another itemset is called a 1-extension of the latter itemset.

Constraints on various measures of significance and interest can be used to select interesting associations and rules. Agrawal et al. (1993) define the measures support and confidence for association rules.

**Definition 1 (Support)** *Support is defined on itemset $Z \subseteq I$ as the proportion of transactions in which all items in $Z$ are found together in the database:*

$$\text{supp}(Z) = \frac{\text{freq}(Z)}{|\mathcal{D}|},$$

*where* freq$(Z)$ *denotes the frequency of itemset $Z$ (number of transactions in which $Z$ occurs) in database $\mathcal{D}$, and $|\mathcal{D}|$ is the number of transactions in the database.*

Confidence is defined for a rule $X \longrightarrow Y$ as the ratio $\text{supp}(X \cup Y)/\text{supp}(X)$. Since confidence is not a frequency constraints we will only discuss support in the following.

An itemset $Z$ is only considered significant and interesting in the association rule framework if the constraint $\text{supp}(Z) \geq \sigma$ holds, where $\sigma$ is a user-specified minimum support. Itemsets which satisfy the minimum support constraint are called *frequent itemsets* since their occurrence frequency surpasses a set frequency threshold, hence the name frequency constraint. Some authors refer to frequent itemsets also as *large itemsets* (Agrawal et al., 1993) or *covering sets* (Mannila et al., 1994).

The rational for minimum support is that items which appear more often in the database are more important since, e.g. in a sales setting they are responsible for a higher sales volume. However, this rational breaks down when some rare but expensive items contribute most to the store's overall earnings. Not finding associations for such items is known as support's rare item problem (Liu et al., 1999). Support also systematically favors smaller itemsets (Seno and Karypis, 2001). By adding items to an itemset the probability of finding such longer itemsets in the database can only decrease or, in rare cases, stay the same. Consequently, longer itemsets are less likely to meet the minimum support. Reducing minimum support to find longer itemsets normally results in an explosion of the number of small itemsets found, which makes this approach infeasible for most applications.

For all but very small or extremely sparse databases, finding all frequent itemsets is computationally very expensive since the search space for frequent itemsets grows exponentially with the number of items. However, the minimum support constraint possesses a special property called *downward closure* (Agrawal and Srikant, 1994) (also called *anti-monotonicity* (Pei et al., 2001)) which can be used to make more efficient search possible. A constraint is downward closed (anti-monotone) if, and only if, for each itemset which satisfies the constraint all subsets also satisfy the constraint. The frequency constraint minimum support is downward closed since if set $X$ is supported at a threshold $\sigma$, also all its subsets $Y \subset X$, which can only have a higher or the same support as $X$, must be supported at the same threshold. This property implies that (a) an itemset can only satisfy a downward closed constraint if all its subsets satisfy the constraint and that (b) if an itemset is found to satisfy a downward closed constraint all its subsets need no inspection since they must also satisfy the constraint. These facts are used by mining algorithms to reduce the search space which is often referred to as *pruning* or finding a border in the lattice representation of the search space.

Driven by support's problems with rare items and skewed item frequency distributions, some researchers proposed alternatives for mining associations. In the following we will review some approaches which are related to this work.

Liu et al. (1999) try to alleviate the rare item problem. They suggest mining itemsets with individual *minimum item support* thresholds assigned to each item. Liu et al. showed that after sorting the items according to their minimum item support a *sorted closure property* of minimum item support can be used to prune the search space. A open research question is how to determine

the optimal values for the minimum item supports, especially in databases with many items where a manual assignment is not feasible.

Seno and Karypis (2001) try to reduce support's tendency to favor smaller itemsets by proposing a minimum support which decreases as a function of itemset length. Since this invalidates the downward closure of support, the authors develop a property called *smallest valid extension,* which can be exploited for pruning the search space. As a proof of concept, the authors present results using a linear function for support. However, an open question is how to choose an appropriate support function and its parameters.

Omiecinski (2003) introduced several alternative interest measures for associations which avoid the need for support entirely. Two of the measures are *any-* and *all-confidence.* Both rely only on the confidence measure defined for association rules. Any-confidence is defined as the largest confidence of a rule which can be generated using all items from an itemset. The author states that although finding all itemsets with a set any-confidence would enable us to find all rules with a given minimum confidence, any-confidence cannot be used efficiently as a measure of interestingness since minimum confidence is not downward closed. The all-confidence measure is defined as the smallest confidence of all rules which can be produced from an set of associated items. Omiecinski shows that a minimum constraint on all-confidence is downward closed and, therefore, can be used for efficient mining algorithms without support.

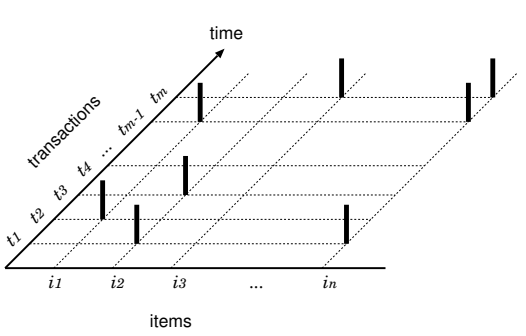
Another family of approaches is based on using statistical methods to mine associations. The main idea is to identify associations as significant deviations from a baseline given by the assumption that items occur statistically independent from each other. The simplest measure to quantify this deviation is *interest* (Brin et al., 1997) which is often also called *lift.* Interest for a rule $X \longrightarrow Y$ is defined as $P(X \cup Y)/(P(X)P(Y))$, where the denominator is the baseline probability, the expected probability of the itemset under independence. Interest is usually calculated by the ratio $r_{obs}/r_{exp}$ which are the observed and the expected occurrence counts of the itemset. The ratio is close to one if the itemsets $X$ and $Y$ occur together in the database as expected under the assumption that they are independent. A value greater than one indicates a positive correlation between the itemsets and values lesser than one indicate a negative correlation. To smooth away noise for low counts in the interest ratio, DuMouchel and Pregibon (2001) developed the empirical Bayes Gamma-Poisson shrinker. However, the interest ratio is not a frequency constraint and does not possess the downward closure property needed for efficient mining.

Silverstein et al. (1998) suggested mining dependence rules using the $\chi^2$ test for independence between items on $2 \times 2$ contingency tables. The authors use the fact that the test statistic can only increase with the number of items to develop mining algorithms which rely on this *upward closure property.* DuMouchel and Pregibon (2001) pointed out that more important than the test statistic is the test's p-value. Due to the increasing number of degrees of freedom of the $\chi^2$ test the p-value can increase or decrease with itemset size, which invalidates the upward closure property. Furthermore, Silverstein et al. (1998) mention that a significant problem of the approach is the normal approximation used in the $\chi^2$ test. This can skew results unpredictably for contingency tables with cells with low expectation.

First steps towards the approach presented in this paper were made with two projects concerned with finding related items for recommendation systems (Geyer-Schulz et al., 2002, 2003). The used algorithms were based on the logarithmic series distribution (LSD) model which is a simplification of the NB model used in this paper. Also the algorithms were restricted to find only 2-itemsets. However, the projects showed that the approach described in this paper produces good results for real-world applications.

# 3 Developing a Model-Based Frequency Constraint

In this section we build on the idea of discovering associated items with the help of observed deviations of co-occurrences from a baseline which is based on independence between all items. This is similar to how interest (lift) uses the expected probability of itemsets under independence to identify dependent itemsets. In contrast to lift and other similar measure, we will not estimate




(a)

items

| transactions | i1 | i2 | i3 | ... | in | size |
|---|---|---|---|---|---|---|
| t1 | 0 | 1 | 0 | ... | 1 | 5 |
| t2 | 1 | 0 | 0 | ... | 0 | 2 |
| t3 | 0 | 1 | 0 | ... | 0 | 1 |
| t4 | 0 | 0 | 0 | ... | 0 | 1 |
| . | . | . | . | . | | . |
| . | . | . | . | . | | . |
| . | . | . | . | . | | . |
| tm-1 | 1 | 0 | 0 | ... | 1 | 3 |
| tm | 0 | 0 | 1 | ... | 1 | 2 |
| freq | 99 | 201 | 7 | ... | 411 | 50614 |

(b)

Figure 1: Representation of an example database as (a) sequence of transactions and (b) the incidence matrix.

the degree of deviation at the level of an individual itemset. Rather, we will evaluate the deviation for the set of all possible 1-extensions of an itemset together to find a local frequency constraint for these extensions. A 1-extension of an $k$ itemset is an itemset of size $k+1$ which is produced by adding an additional item to the $k$-itemset.

## 3.1 A Simple Stochastic Baseline Model

A suitable stochastic item occurrence model for the baseline frequencies needs to describe the occurrence of independent items with different usage frequencies in a robust and mathematically tractable way. For the model we consider the occurrence of items $I = \{i_1, i_2, \ldots, i_n\}$ in a database with a fixed number of $m$ transactions. An example database is depicted in Fig. 1. For the example we use $m = 20,000$ transactions and $n = 500$ items. To the left we see a graphical representation of the database as a sequence of transactions over time. The transactions contain items depicted by the bars at the intersections of transactions and items. The typical representation used for data mining is the $m \times n$ incidence matrix in Fig. 1(b). Each row sum represents the size of a transaction and the column sums are the frequencies of the items in the database. The total sum represents the number of incidences (item occurrences) in the database. Dividing the number of incidences by the number of transactions gives the average transaction size (for the example, $50,614/20,000 = 2.531$) and dividing the number of incidences by the number of items gives the average item frequency ($50,614/500 = 101.228$).

In the following we will model the baseline for the distribution of the items' frequency counts *freq* in Fig. 1(b). For the baseline we suppose that each item in the database follows an independent (homogeneous) Poisson process with an individual latent rate $\lambda$. Therefore, the frequency for each item in the database is a value drawn from the Poisson distribution with its latent rate. We also assume that the individual rates are randomly drawn from a suitable distribution defined by the continuous random variable $\Lambda$. Then the probability distribution of $R$, a random variable which gives the number of times an arbitrarily chosen item occurs in the database, is given by

$$Pr[R = r] = \int_0^\infty \frac{e^{-\lambda}\lambda^r}{r!} dG_\Lambda(\lambda),\ r = 0, 1, 2, ...,\ \lambda > 0. \tag{1}$$

This Poisson mixture model results from the continuous mixture of Poisson distributions with rates following the mixing distribution $G_\Lambda$.

Heterogeneity in the occurrence frequencies between items is accounted for by the form of the mixing distribution. A commonly used and very flexible mixing distribution is the Gamma distribution with the density function

$$g_\Lambda(\lambda) = \frac{e^{-\lambda/a}\lambda^{k-1}}{a^k \Gamma(k)},\ a > 0,\ k > 0, \tag{2}$$

where $a$ and $k$ are the distribution's scaling and the shape parameters.

Integrating Eq. (1) with (2) is known to result in the negative binomial (NB) distribution (see, e.g., Johnson et al. (1993)) with the probability distribution

$$Pr[R = r] = (1 + a)^{-k} \frac{\Gamma(k + r)}{\Gamma(r + 1)\Gamma(k)} \left(\frac{a}{1 + a}\right)^r , \; r = 0, 1, 2, ... \tag{3}$$

This distribution gives the probability that we see arbitrarily chosen items with a frequency of $r = 0, 1, 2, ...$ in the database. The average frequency of the items in the database is given by $a/k$ and $Pr[R = 0]$ represents the proportion of available items which never occurred during the time the database was recorded.

Once the parameters $k$ and $a$ are known, the expected probabilities of finding items with a frequency of $r$ in the database can be efficiently computed by calculating the probability of the zero class by $Pr[R = 0] = (1 + a)^{-k}$ and then using the recursive relationship (see Johnson et al. (1993))

$$Pr[R = r + 1] = \frac{k + r}{r + 1} \; \frac{a}{1 + a} \; Pr[R = r]. \tag{4}$$

Although, the NB model (often also called Gamma-Poisson model) simplifies reality considerably with its assumed Poisson processes and the Gamma mixing distribution, it is widely and successfully applied for accident statistics, birth-and-death processes, economics, library circulation, market research, medicine, and military applications (Johnson et al., 1993).

## 3.2 Fitting the Model to Transaction Data Sets

The parameters of the NB distribution can be estimated by several methods including the method of moments, maximum likelihood, and others (Johnson et al., 1993). All methods need the item frequency counts *freq* for the estimation. This information is obtained by passing over the database once. Since this counts are necessary to calculate the item support needed by most mining algorithms, the overhead can be saved later on when itemsets are mined.

Particularly simple is the method of moments where $\tilde{k} = \bar{r}^2/(s^2 - \bar{r})$ and $\tilde{a} = \bar{r}/\tilde{k}$ can be directly computed from the observed mean $\bar{r} = \text{mean}(\textit{freq})$ and variance $s^2 = \text{var}(\textit{freq})$ of the item occurrence frequencies. However, with empirical data we face two problems: (a) the zero-class (available items which never occurred in the database) are often not observable and (b) as reported for other applications of the NB model, in real-world data often exist a small number of items with a too high frequency to be covered by the Gamma mixing distribution used in the model.

A way to obtain the missing zero-class is to subtract the number of observed items from the total number of items which were available at the time the database was recorded. The number of available items can be obtained from the provider of the database. If the total number of available items is unknown, the size of the zero-class can be estimated together with the parameters of the NB distribution. The standard procedure for this type of estimation problem is the *Expectation Maximization (EM)* algorithm (Dempster et al., 1977). This procedure iteratively estimates missing values using the observed data and the model using intermediate values of the parameters, and then uses the estimated data and the observed data to update the parameters for the next iteration. The procedure stops when the parameters stabilize. For our estimation problem the procedure is computationally very inexpensive. Each iteration involves only to calculate $n(1+\tilde{a})^{-\tilde{k}}$ to estimate the count for the missing zero-class and then applying the method of moments (see above) to update the parameter estimates $\tilde{a}$ and $\tilde{k}$. As we will see in the examples later in this section, the EM algorithm usually only needs a small number of iteration to estimate the needed parameters. Therefore, the computational cost of estimation is insignificant compared to the time needed to count the item frequencies in the database.

The second estimation problem are outliers with too high frequencies. These outliers will distort the mean and the variance and thus will lead to a model which grossly overestimates the probability of seeing items with high frequencies. For a more robust estimate, we can trim a

Table 1: Characteristics of the used data sets.

| | **WebView-1** | **POS** | **Artif-1** |
|---|---|---|---|
| Transactions | 59,602 | 515,597 | 100,000 |
| Avg. trans. size | 2.5 | 6.5 | 10.1 |
| Median trans. size | 1 | 4 | 10 |
| Distinct items | 497 | 1,657 | 844 |

suitable percentage of the items with the highest frequencies. A suitable percentage can be found by visual comparison of the empirical data and the estimated model or by minimizing the $\chi^2$-value of the goodness-of-fit test.

To demonstrate that the parameters for the developed baseline model can be estimated for data sets, we use the two e-commerce data sets *WebView-1* and *POS* provided by Blue Martini Software for the KDD Cup 2000 (Kohavi et al., 2000) and an artificial data set, *Artif-1*. WebView-1 contains several months of clickstream data from an e-commerce Web site where each transaction consists of the product detail page views during a session. POS is a point-of-sale data set containing several years of data. Artif-1 is better known as *T10I4D100K*, a widely used artificial data set generated by the procedure described by Agrawal and Srikant (1994).

Table 1 contains the basic characteristics of the data sets. The data sets differ in the number of items and the average number of items per transactions. The real-world data sets show that their median transaction size is considerably smaller than their mean which indicates that the distribution of transaction lengths is skewed with many very short transactions and some very long transactions. The artificial data set does not show this property. For a comparison of the data sets' properties and their impact on the effectiveness of different association rule mining algorithms we refer to Zheng et al. (2001)[1].

Before we estimated the model parameters with the EM algorithm, we discarded the first 10,000 transactions for WebView-1 since a preliminary data screening showed that the average transaction size and the number of items used in these transactions is more volatile and significantly smaller than for the rest of the data set. This might indicate that at the beginning of the database there were still major changes made to the Web shop (e.g., reorganizing the Web site, or adding and removing promotional items). POS and Artif-1 do not show such effects. To remove outliers (items with too high frequencies), we used visual inspection of the item frequency distributions and the fitted models for a range of trimming values (between 0 and 10%). To estimate the parameters for the two real-world data sets we chose to trim 2.5% of the items with the highest frequency. The synthetic data set does not contain outliers and therefore no trimming was necessary.

In Table 2, we summarize the results of the fitting procedure for samples of size 20,000 transactions from the three data sets. To check whether the model provides a useful approximation for the data, we used the $\chi^2$ goodness-of-fit test. As recommended for the test, we combined classes so that in no class the expected count is below 5 and used a statistical package to calculate the p-values. For all data sets we found high p-values ($\gg 0.05$) which indicates that no significant difference between the data and the corresponding models could be found and the model fits the data sets reasonably well.

To evaluate the stability of the model parameters, we estimated the parameters for samples of different sizes. We expect that the shape parameter $k$ is independent of the sample size while the scale parameter $a$ depends linearly on the sample size. This can be simply explained by the fact that, if we, observe the Poisson process for each item, e.g., twice as long, we have to double the latent parameter $\lambda$ for each process. For the Gamma mixing distribution this means that the scale parameter $a$ must be double. Consequently, $a$ divided by the size of the sample should be constant.

[1] Although the artificial data set in this paper and in Zheng et al. (2001) were produced using the same generator (available at http://www.almaden.ibm.com/software/quest/Resources/), there are minimal variations due to differences in the used random number generator initialization.

Table 2: The fitted NB models using samples of 20,000 transactions.

| | **WebView-1** | **POS** | **Artif-1** |
|---|---|---|---|
| Observed items | 342 | 1,153 | 843 |
| Trimmed items | 9 | 29 | 0 |
| Item occurrences | 33,802 | 87,864 | 202,325 |
| EM iterations | 3 | 29 | 3 |
| Estim. zero-class | 6 | 2,430 | 4 |
| Used items ($\tilde{n}$) | 339 | 3,554 | 847 |
| $\bar{r}$ | 99.711 | 24.723 | 238.873 |
| $s^2$ | 11,879.543 | 9,630.206 | 59,213.381 |
| $\tilde{k}$ | 0.844 | 0.064 | 0.968 |
| $\tilde{a}$ | 118.141 | 386.297 | 242.265 |
| $\chi^2$ p-value | 0.540 | 0.101 | 0.914 |

Table 3: Estimates for the NB-model using samples of different sizes.

| Name | Sample size | $\tilde{k}$ | $\tilde{a}$ | $\tilde{a}$ per transaction | $\tilde{n}$ |
|---|---|---|---|---|---|
| **WebView-1** | 10,000 | 0.933 | 58.274 | 0.0058 | 325 |
| **WebView-1** | 20,000 | 0.844 | 118.140 | 0.0059 | 339 |
| **WebView-1** | 40,000 | 0.868 | 218.635 | 0.0055 | 395 |
| **POS** | 10,000 | 0.060 | 178.200 | 0.0178 | 3,666 |
| **POS** | 20,000 | 0.064 | 386.300 | 0.0193 | 3,554 |
| **POS** | 40,000 | 0.064 | 651.406 | 0.0163 | 3,552 |
| **Artif-1** | 10,000 | 0.975 | 123.313 | 0.0123 | 845 |
| **Artif-1** | 20,000 | 0.968 | 242.265 | 0.0121 | 847 |
| **Artif-1** | 40,000 | 0.967 | 493.692 | 0.0123 | 846 |

Table 3 gives the parameter estimates (also $a$ per transaction) and the estimated total number of items $n$ (observed items + estimated zero class) for samples of sizes $10,000$ to $40,000$ transactions from the three databases. The estimates for the parameters $k$, $a$ per transaction, and the number of items $n$ generally show only minor variations over different sample sizes of the same data set. We analyzed the reason for the high jump of the estimated number of items from 339 for $20,000$ transactions to 395 for $40,000$ transactions in WebView-1. We found evidence in the database that after the first $20,000$ transactions the number of different items in the database starts to grow by about 10 items every $5,000$ transactions. However, this fact does not seem to influence the stability of the estimates of the parameters $k$ and $a$. The stability enables us to use model parameters estimated for one sample size for samples of different sizes.

Applied to associations, Eq. (3) in the section above gives the probability distribution of observing single items (1-itemsets) with a frequency of $r$. Let $\sigma^{freq} = \sigma m$, where $m$ is the number of transactions in the database, be the frequency threshold equivalent to the minimum support $\sigma$. Then the expected number of 1-itemsets which satisfy the frequency threshold $\sigma^{freq}$ is given by

$$nPr[R \geq \sigma^{freq}],$$

where $n$ is the number of available items. In Fig. 2 we show for the data sets the number of frequent 1-itemsets predicted by the fitted models (solid line) and the actual number (dashed line) by a varying minimum support constraint. For easier comparison we show relative support for the plots. In all three plots we can see how the models fit the skewed support distributions.

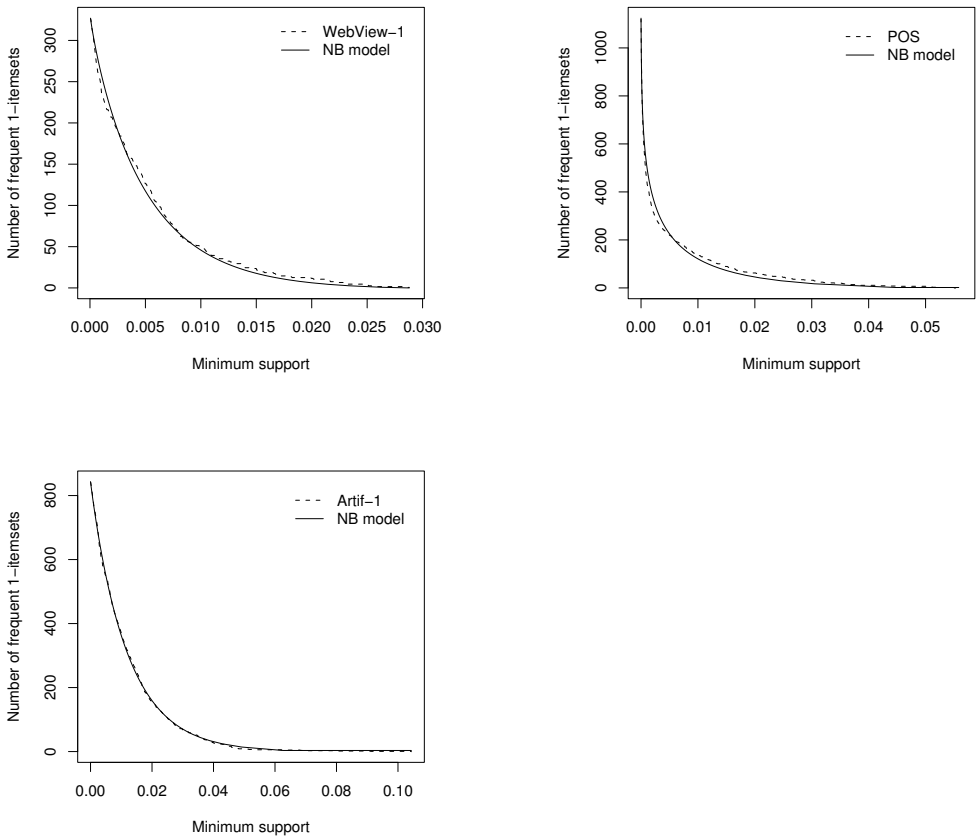



Figure 2: Actual versus predicted number of frequent items by minimum support.

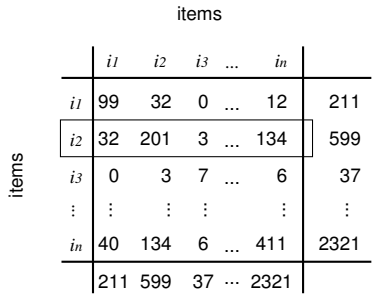



Figure 3: A $n \times n$ matrix for counting 2-itemsets in the database.

### 3.3 Extending the Baseline Model to $k$-Itemsets

After only considering 1-itemsets, we show how the model developed above can be extended to provide a baseline for the distribution of support over all possible 1-extensions of an itemset.

We start with 2-itemsets before we generalize to itemsets of arbitrary length. Fig. 3 shows an example of the co-occurrence frequencies of all items (occurrence of 2-itemsets) in transactions organized as an $n \times n$ matrix. The matrix is symmetric around the main diagonal which contains the count frequencies of the individual items $\text{freq}(i_1), \text{freq}(i_2), \ldots, \text{freq}(i_n)$. By adding the count values for each row or for each column, we get in the margins of the matrix the number of incidences in all transactions which contain the respective item.

For example, to build the model for all 1-extensions of item $i_2$, we only need the information in the box in Fig. 3. It contains the frequency counts for all 1-extensions of $i_2$ plus $\text{freq}(i_2)$ in cell $(2, 2)$. Note, that these counts are only affected by transactions which contain item $i_2$. If we select all transactions which contain item $i_2$, we get a sample of size $\text{freq}(i_2) = 201$ from the database. For the baseline model with only independent items, the co-occurrence counts in the sample follow again Poisson processes. Following the model in Section 3.1 we can obtain a new random variable $R_{i_2}$ which models the occurrences of an arbitrarily chosen 1-extensions of $i_2$.

After presenting the idea for the 1-extensions of a single item, we now turn to the general case of building a baseline model for all 1-extensions of an association $l$ of arbitrary length. We denote the number of items in $l$ by $k$. Thus $l$ is a $k$-itemset for which exactly $n - k$ different 1-extensions exist. All 1-extensions of $l$ can be generated by joining $l$ with all possible single items $c \in I \setminus l$. The items $c$ will be call candidate items. In the baseline model all candidate items are independent from the items in $l$. Consequently, the set of all transactions which contain $l$ represent a sample of size $\text{freq}(l)$, which is random with respect to the candidate items. Following the developed model also the baseline for the number of candidate items with frequency $r$ in the sample has a NB distribution. More precisely, the counts for the 1-extensions of $l$ can be modeled by a random variable $R_l$ with the probability distribution

$$Pr[R_l = r] = (1 + a_l)^{-k} \frac{\Gamma(k + r)}{\Gamma(r + 1)\Gamma(k)} \left( \frac{a_l}{1 + a_l} \right)^r \quad for\ r = 0, 1, 2, ... \tag{5}$$

The distribution's shape parameter $k$ is not affected by sample size and we can use the estimate $\tilde{k}$ from the database. However, the parameter $a$ is linearly dependent on the sample size (see Section 3.2 above). To obtain $a_l$, we have to rescale $\tilde{a}$, estimated from the database, for the sample size $\text{freq}(l)$.

To rescale $a$ we could use the proportion of the transactions in the sample relative to the size of the database which was used to estimate $\tilde{a}$. In Section 3.2 above, we showed that for estimating the parameter for different sample sizes gives a stable value for $\tilde{a}$ per transaction. A problem with applying transaction-based rescaling is that the more items we include in $l$, the smaller the number of remaining items per transaction gets. This would reduce the effective transaction length and the estimated model would not be applicable. Therefore, we will ignore the concept of transactions for the following and treat the data set as a series of incidences (occurrences of items). For the

baseline model this is unproblematic since the mixture model never used the information that items occur together in transactions. At the level of incidences, we can rescale $a$ by the proportion of incidences in the sample relative to the total number of incidences in the database from which we estimated the parameter. We do this in two steps:

1. We calculate $\tilde{a}'$, the parameter per incidence, by dividing the parameter obtained from the database by the total number of incidences in the database.

$$\tilde{a}' = \frac{\tilde{a}}{\sum_{t \in \mathcal{D}} |t|} \tag{6}$$

2. We rescale the parameter for itemset $l$ by multiplying $\tilde{a}'$ with the number of incidences in the sample (transactions which contain $l$) excluding the occurrences of the items in $l$.

$$\tilde{a}_l = \tilde{a}' \sum_{\{t \in \mathcal{D} | t \supset l\}} |t \setminus l| \tag{7}$$

For item $i_2$ in the example in Fig. 3, the rescaled parameter can be easily calculated from the sum of incidences for the item (599) in the $n \times n$ matrix together with the the sum of incidences $(50,614)$ in the total incidence matrix (see Fig. 1 above in Section 3.1) by $\tilde{a}' = \tilde{a}/50614$ and $\tilde{a}_{i_2} = \tilde{a}' \cdot 599$.

## 3.4 Deriving a Model-Based Frequency Constraint for NB-Frequent Itemsets

The NB distribution with the parameters rescaled for itemset $l$ provides a baseline for the frequency distribution of the candidate items in the transactions which contain $l$, i.e., the number of different itemsets $l \cup \{c\}$ with $c \in I \setminus l$ we would expect per support count, if all items were independent. If in the database some item candidates are related to the items in $l$, the transactions that contain $l$ cannot be considered a random sample for these items. These related items will have a higher frequency in the sample than expected by the baseline model.

To find a set $L$ of non-random 1-extensions of $l$ (extensions with item candidates with a too high co-occurrence frequency), we need to identify a frequency threshold $\sigma_l^{freq}$, where accepting item candidates with a frequency count $r \geq \sigma_l^{freq}$ separates associated items best from items which co-occur often by pure chance. For this task we need to define a quality measure on $L$, the set of accepted 1-extensions. *Precision* is a possible quality measure which is widely used by the machine learning community (Kohavi and Provost, 1988) and is defined as the proportion of correctly predicted positive cases in all predicted positive cases. Using the baseline model and observed data, we can predict precision for different values of the frequency threshold.

**Definition 2 (Predicted precision)** *Let $L$ be the set of all 1-extensions of a known association $l$ which are generated by joining $l$ with all candidate items $c \in I \setminus l$ which co-occurrence with $l$ in at least $\rho$ transactions. For set $L$ we define the predicted precision as*

$$\text{precision}_l(\rho) = \begin{cases} (o_{[r \geq \rho]} - e_{[r \geq \rho]})/o_{[r \geq \rho]} & \text{if } o_{[r \geq \rho]} \geq e_{[r \geq \rho]} \text{ and } o_{[r \geq \rho]} > 0 \\ 0 & \text{otherwise.} \end{cases} \tag{8}$$

*$o_{[r \geq \rho]}$ is the observed and $e_{[r \geq \rho]}$ is the expected number of candidate items which have a co-occurrence frequency with itemset $l$ of $r \geq \rho$. The observed number is calculated as the sum of observations with count $r$ by $o_{[r \geq \rho]} = \sum_{r=\rho}^{r_{max}} o_r$, where $r_{max}$ is the highest observed co-occurrence. The expected number is given by the baseline model as $e_{[r \geq \rho]} = (n - |l|)Pr[R_l \geq \rho]$, where $n - |l|$ is the number of possible candidate items for pattern $l$.*

Predicted precision together with a precision threshold $\pi$ can be used to form a model-based constraint on accepted associations. The smallest possible frequency threshold for 1-extensions of $l$, which satisfies the set minimum precision threshold $\pi$, can be found by

$$\sigma_l^{freq} = \text{argmin}_\rho\{\text{precision}_l(\rho) \geq \pi\}. \tag{9}$$

The set of the chosen candidate items for $l$ is then

$$C_l = \{c \in I \setminus l | \text{freq}(l \cup \{c\}) \geq \sigma_l^{freq}\},$$

and the set of accepted associations is

$$L = \{l \cup \{c\} | c \in C_l\}.$$

The predicted error rate for using a threshold $\sigma_l^{freq}$ is given by $1 - \text{precision}_l(\sigma_l^{freq})$. A suitable selection criterion for a count threshold is to allow only a percentage of falsely accepted associations. For example, if we need for an application all rules with the antecedent $l$ and a single item as the consequent and the maximum number of acceptable spurious rules is 5%, we can find all 1-extension of $l$ and use a minimum precision threshold of $\pi = 0.95$.

Table 4 contains an example for the model-based frequency constraint using data from the WebView-1 database. We analyze the 1-extensions of itemset $l = \{10311, 12571, 12575\}$ at a minimum precision threshold of 95%. The estimates for $n$, $k$ and $a$ are taken from Table 2 in Section 3.2. Parameter $a$ is rescaled to $a_l = 1.164$ using Eqs. (6) and (7) in the previous section. Column $o$ contains the observed number of items with a co-occurrence frequency of $r$ with $l$. The value at $r = 0$ is in parentheses since it is not directly observable. It was calculated as the difference between the estimated number of available candidate items ($n - |l|$) and the number of observed items ($o_{[r>0]}$). Column $e$ contains the expected frequencies calculated with the model. To find the frequency threshold $\sigma_l^{freq}$, the precision function $\text{precision}_l(\rho)$ in Eq. (8) is evaluated starting with $\rho = r_{max}$ (18 in the example in Table 4) and $\rho$ is reduced till we get a predicted precision value which is below the minimum precision threshold of $\pi = 0.95$. The found frequency threshold is then the last value for $r$, which produced a precision above the threshold (in the example at $r = 11$). After the threshold is found, there is no need to evaluate the rest of the precision function with $r < 10$. All candidate items with a co-occurrence frequency greater than the found threshold are selected. For the example in Table 4, this gives a set of 6 chosen candidate items.

There exists an interesting connection to the confidence measure for the way an individual frequency threshold (minimum support) is chosen for all 1-extensions of an itemset.

**Theorem 1** *Let $l$ be an itemset and let $c \in I \setminus l$ be the set of candidate items which form together with $l$ all 1-extensions of $l$. For each possible minimum support $\sigma_l$ on the 1-extensions of $l$, a minimum confidence threshold $\gamma_l$ on the rules $l \longrightarrow \{c\}$ exists, which results in an equivalent constraint. That is, there always exist pairs of values for $\sigma_l$ and $\gamma_l$ were the following holds:*

$$\text{supp}(l \cup \{c\}) \geq \sigma_l \Leftrightarrow \text{conf}(l \longrightarrow \{c\}) \geq \gamma_l.$$

**Proof 1** *With $\text{conf}(l \longrightarrow \{c\})$ defined as $\text{supp}(l \cup \{c\})/\text{supp}(l)$ we can rewrite the right-hand side constraint as $\text{supp}(l \cup \{c\})/\text{supp}(l) \geq \gamma_l$. Since $\text{supp}(l)$ is a positive constant for all considered rules, we get the equality $\gamma_l = \sigma_l/\text{supp}(l)$ by substitution.* □

As an example, suppose a database contains $20,000$ transactions and the analyzed itemset $l$ is contained in 1600 transactions which gives $supp(l) = 1600/20,000 = 0.08$. If we require the candidate items $c$ to have a co-occurrence frequency with $l$ of at least $\text{freq}(l \cup \{c\}) \geq 1200$, we use in fact a minimum support of $\sigma_l = 1200/20,000 = 0.06$. All rules $l \longrightarrow \{c\}$ which can be constructed for the supported itemsets $l \cup \{c\}$ will have at least a confidence of $\gamma_l = 0.06/0.08 = 0.75$.

The aim of developing the model-based frequency constraint is to find as many non-spurious associations as possible in a data base, given a precision threshold. After we introduced the model-based frequency constraint for 1-extensions of a single itemset, we now extend the view to the whole

Table 4: An example for finding the frequency threshold at $\pi = 0.95$ (found at $r = 11$).

| $r$ | $o$ | $e$ | precision($r$) |
|---|---|---|---|
| 0 | (183) | 176.71178 | - |
| 1 | 81 | 80.21957 | - |
| 2 | 48 | 39.78173 | - |
| 3 | 13 | 20.28450 | - |
| 4 | 6 | 10.48480 | - |
| 5 | 0 | 5.46345 | - |
| 6 | 1 | 2.86219 | - |
| 7 | 0 | 1.50516 | - |
| 8 | 1 | 0.79378 | - |
| 9 | 0 | 0.41955 | - |
| 10 | 0 | 0.22214 | 0.92108 |
| 11 | 2 | 0.11779 | 0.95811 |
| 12 | 1 | 0.06253 | 0.96661 |
| 13 | 1 | 0.03323 | 0.97632 |
| 14 | 1 | 0.01767 | 0.98109 |
| 15 | 0 | 0.00941 | 0.97986 |
| 16 | 0 | 0.00501 | 0.98927 |
| 17 | 0 | 0.00267 | 0.99428 |
| 18 | 1 | 0.00305 | 0.99695 |

itemset lattice. For this purpose, we need to find a suitable search strategy which enables us to traverse the itemset lattice efficiently, i.e. to prune parts of the search space which only contain itemsets which are not of interest. For frequent itemset mining, the downward closure property of support is exploited for this purpose. Unfortunately, the model-based frequency constraint does not possess such a property. However, we can develop several search strategies. A straight forward solution is to use an apriori-like level-wise search strategy (starting with 1-itemsets) and in every level $k$ we only expand itemsets which passed the frequency constraint at level $k-1$. This strategy suffers from a problem with candidate items which are extremely frequent in the data base. For such a candidate item, we will always observe a high co-occurrence count with any, even unrelated itemsets. The result is that itemsets which include a frequent but unrelated item are likely to be used in the next level of the algorithm and possibly will be expanded even further. In transaction data bases with a very skewed item frequency distribution this leads to many spurious associations and combinatorial explosion.

Alternatively, since each $k$-itemset can be produced from $k$ different $(k-1)$-subsets (checked at level $k-1$) plus the corresponding candidate item, it is also possible to require that for all $(k-1)$-subsets the corresponding candidate item passes the frequency constraint. This strategy makes intuitively sense since for associated items one expects that each item in the set is associated with the rest of the itemsets and thus should pass the constraint. It also solves the problem with extremely frequent candidate items since it is very unlikely that all unrelated and less frequent items pass by chance the potentially high frequency constraint for the extremely frequent item. Furthermore, this strategy prunes the search space significantly since an itemset is only used for expansion if all subsets passed the frequency constraint. However, the strategy has a problem with including a relatively infrequent item into a set consisting of more frequent items. It is less likely that the infrequent item as the candidate item meets the frequency constraint set by the more frequent itemset, even if it is related. Therefore it is possible that itemsets consisting of related items with varying frequencies are missed.

A third solution is to used a trade-off between the problems and pruning effects of the two search strategies by requiring for a fraction $\theta$ (between one and all) of the subsets with their candidate items to pass the frequency constraint. We now formally introduce the concept of

*NB-frequent itemsets* which can be used to implement all three solutions:

**Definition 3 (NB-frequent itemset)** *A $k$-itemset $l'$ with $k > 1$ is a NB-frequent itemset if, and only if, at least a fraction $\theta$ (at least one) of its $(k-1)$-subsets $l \in \{l' \setminus \{c\} | c \in l'\}$ are NB-frequent itemsets and satisfy* $\text{freq}(l \cup \{c\}) \geq \sigma_l^{freq}$. *The frequency thresholds $\sigma_l^{freq}$ are individually chosen for each itemset $l$ using Eq. (9) with a user-specified precision threshold $\pi$. All itemsets of size* 1 *are per definition NB-frequent.*

This definition clearly shows that NB-frequency in general is not downward closed since only a fraction $\theta$ of the $(k-1)$-subsets of a NB-frequent set of size $k$ are required to be also NB-frequent. Only the special case with $\theta = 1$ offers downward closure, but since the definition of NB-frequency is recursive, we can only determine if an itemset is NB-frequent if we first evaluate all its subsets. However, the definition enables us to build algorithms which find all NB-frequent itemsets in a bottom-up search (expanding from 1-itemsets) and even to prune the search space. The magnitude of pruning depends on the setting for parameter $\theta$.

Conceptually, mining NB-frequent itemsets with the extreme values 0 and 1 for $\theta$ is similar to using Omiecinski's (2003) any-confidence and all-confidence. In Theorem 1 we showed that the minimum support $\sigma_l$ chosen for NB-frequent itemsets $l \cup \{c\}$ is equivalent to choosing a minimum on confidence $\gamma_l = \sigma_l / \text{supp}(l)$ for the rules $l \longrightarrow \{c\}$. An itemset passes a threshold on any-confidence if at least one rule can be constructed from the itemset which has a confidence value greater or equal of the threshold. This is similar to mining NB-frequent itemsets with $\theta = 0$, where to accept itemset $l \cup \{c\}$ a single combination $\text{conf}(l \longrightarrow \{c\}) \geq \gamma_l$ suffices.

For all-confidence, all rules which can be constructed from an itemset must have a confidence greater or equal than a threshold. This is similar to mining NB-frequent itemsets with $\theta = 1$ where we require $\text{conf}(l \longrightarrow \{c\}) \geq \gamma_l$ for all possible combination. Note, that in contrast to all- and any-confidence, we do not use a single threshold for mining NB-frequent itemsets, but an individual threshold is chosen by the model for each itemset $l$.

# 4 A Mining Algorithm for NB-Frequent Itemsets

In this section we develop an algorithm using a depth-first search strategy to mine all NB-frequent itemset in a database. The algorithm implements the candidate item selection mechanism of the model-based frequency constraint in the NB-Select function. The function's pseudocode is presented in Table 5. It is called for each found association $l$ and gets count information of all 1-extensions of $l$, characteristics of the data set ($n$, $\tilde{k}$, $\tilde{a}'$), and the user-specified precision threshold $\pi$. NB-Select returns the set of selected candidate items for $l$.

Table 6 contains the pseudocode for NB-DFS, the main part of the mining algorithm. The algorithm uses a similar structure as *DepthProject,* an algorithm to efficiently find long maximal itemsets (Agarwal et al., 2000). NB-DFS is started with NB-DFS($\emptyset, \mathcal{D}, n, \tilde{k}, \tilde{a}', \pi, \theta$) and recursively calls itself with the next analyzed itemset $l$ and its conditional database $\mathcal{D}_l$ to mine for subsequent NB-frequent supersets of $l$. The conditional database $\mathcal{D}_l$ is a sub-database which only contains transactions which contain $l$. NB-DFS scans all transactions in the conditional database to create the data structure $\mathcal{L}$ which stores the count information for the candidate items and is needed by NB-Select. New NB-frequent itemsets are generated with the NB-Gen function which will be discussed later. The algorithm stops when all NB-frequent itemsets are found.

Compared to a level-wise breadth-first search algorithm, e.g. Apriori, the depth-first algorithm uses significantly more passes over the database. However, every time only a conditional database is scanned. This conditional database only contains the transactions that include the itemset which is currently expanded. Note, that this conditional database contains all information needed to find all NB-frequent supersets of the expanded itemset. As this itemset grows longer, the conditional database gets quickly smaller. If the original database is too large to fit into main memory, a conditional databases will fit into the memory after the expanded itemset grew in size. This will make the subsequent scans very fast.

Table 5: Pseudocode for selecting candidate items for the NB-frequent itemset $l$ using a minimum precision constraint.

**function NB-Select**$(l, \mathcal{L}, n, \tilde{k}, \tilde{a}', \pi)$:

$l$ = the itemset for which candidate items are selected

$\mathcal{L}$ = a data structure which holds all candidate items $c$ together with the associated counts $c.count$

$n$ = the total number of available items in the database

$\tilde{k}, \tilde{a}'$ = estimated parameters for the database

$\pi$ = user-specified precision threshold

1. $r_{max} = max\{c.count | c \in \mathcal{L}\}$
2. $rescale = sum\{c.count | c \in \mathcal{L}\}$
3. **foreach** count $c.count \in \mathcal{L}$ **do** $o_{[c.count]}$++
4. $\rho = r_{max}$
5. **do**
6. precision $= 1 - (n - |l|)Pr[R_l \geq \rho | k = \tilde{k}, a = \tilde{a}' rescale] / \sum_{r=\rho}^{r_{max}} o_r$
7. **while** (precision $\geq \pi \wedge \rho-- > 0$)
8. $\sigma^{\text{freq}} = \rho + 1$
9. **return** $\{c \in \mathcal{L} | c.count \geq \sigma^{\text{freq}}\}$

The generation function NB-Gen has a similar purpose as candidate generation in support-based algorithms: It controls what parts of the search space are pruned. Therefore, a suitable candidate generation strategy is crucial for the performance of the mining algorithm. As already discussed, NB-frequency does not possess the downward closure property which would allow pruning in the same way as for minimum support. However, the definition of NB-frequent itemsets provides us with a way to prune the search space. From the definition we know that in order for a $k$-itemset to be NB-frequent at least a proportion $\theta$ of its $(k-1)$-subset have to be NB-frequent and produce the itemset together with an accepted candidate item. Since for each $k$-itemset exist $k$ different subsets of size $k-1$, we only need to continue the depth-first search for the $k$-itemset, for which we already found at least $k\theta$ NB-frequent $(k-1)$-subset. This has a pruning effect on the search space size.

We present the pseudocode for the generation functions in Table 7. The function is called for each found NB-frequent itemset $l$ individually and gets the set of accepted candidate items and the parameter $\theta$. To enforce $\theta$ for the generation of a new NB-frequent itemset $l'$ of size $k$, we need the information of how many different NB-frequent subsets of size $k-1$ also produce $l'$. And, at the same time, we need to make sure that no part of the lattice is traversed more than once. Other depth-first mining algorithms (e.g., FP-Growth or DepthProject) solve this problem by using special representations of the database (frequent pattern tree structures (Han et al., 2004) or a lexicographic tree (Agarwal et al., 2000)). These representations ensure that no part of the search space can be traversed more than once. However, these techniques only work for frequent itemsets using the downward closed minimum support constraint. To enforce the fraction $\theta$ for NB-frequent itemsets and to ensure that itemsets in the lattice are only traversed once by NB-DFS, we use a global repository $\mathcal{R}$. This repository is used to keep track of the number of times a candidate itemset was already generated and of the itemsets which were already traversed. This solution was inspired by the implementation of closed and maximal itemset filtering implemented for the *Eclat* algorithm by Borgelt (2003).

Table 6: Pseudocode for a recursive depth-first search algorithm for NB-frequent itemsets.

**algorithm NB-DFS**$(l, \mathcal{D}_l, n, \tilde{k}, \tilde{a}', \pi, \theta)$:

$l$ = a NB-frequent itemset

$\mathcal{D}_l$ = a conditional database only containing transactions which include $l$

$n$ = the number of all available items in the database

$\tilde{k}$, $\tilde{a}'$ = estimated parameters for the database

$\pi$ = user-specified precision threshold

$\theta$ = user-specified required fraction of NB-frequent subsets

$\mathcal{L}$ = data structure for co-occurrence counts

1. $\mathcal{L} = \emptyset$
2. **foreach** transaction $t \in \mathcal{D}_l$ **do begin**
3. **foreach** candidate item $c \in t \setminus l$ **do begin**
4. **if** $c \in \mathcal{L}$ **then** $c.count$++
5. **else** add new counter $c.count = 1$ to $\mathcal{L}$
6. **end**
7. **end**
8. **if** $l \neq \emptyset$ **then** selected candidates $C =$ NB-Select$(l, \mathcal{L}, n, \tilde{k}, \tilde{a}', \pi)$
9. **else** initial run candidates are $C = \{c \in \mathcal{L}\}$
10. delete or save data structure $\mathcal{L}$
11. $L =$ NB-Gen$(l, C, \theta)$
12. **foreach** new NB-frequent itemset $l' \in L$ **do begin**
13. $\mathcal{D}_{l'} = \{t \in \mathcal{D}_l | t \supseteq l'\}$
14. $L = L \cup$ NB-DFS$(l', \mathcal{D}_{l'}, n, \tilde{k}, \tilde{a}', \pi, \theta)$
15. **end**
16. **return** $L$

# 5 Experimental Results

In this section we analyze the properties and the effectiveness of mining NB-frequent itemsets. To compare the performance of NB-frequent itemsets with existing methods we use frequent itemsets and itemsets generated using all-confidence as benchmarks. We chose frequent itemsets since a single support value represents the standard in mining association rules. All-confidence was chosen because of its promising properties and its conceptual similarity with mining NB-frequent itemsets with $\theta = 1$.

## 5.1 Investigation of the Itemset Generation Behavior

First, we examine how the number of the NB-frequent itemsets found by the model-based algorithm depends on the parameter $\theta$, which controls the magnitude of pruning, and on the precision parameter $\pi$. For the generation function we use the settings with no and with maximal pruning ($\theta = 0$, $\theta = 1$) and the intermediate value $\theta = 0.5$ which reduces the problems with itemsets containing items with extremely different frequencies (see discussion in section 3.4). Generally, we vary the parameter $\pi$ for NB-Select between 0.5 and 0.999. However, since combinatorial explosion limits the range of practicable settings, depending on the data set and the parameter $\theta$, some values of $\pi$ are omitted.

We report the influence of the different settings for $\theta$ and $\pi$ on the three data sets already

Table 7: Pseudocode for the generation function for NB-frequent itemsets.

**function NB-Gen**$(l, C, \theta)$:

$l$ = a NB-frequent itemset

$C$ = the set of candidate items chosen by NB-Select for $l$

$\theta$ = a user-specified parameter

$\mathcal{R}$ = a global repository containing for each traversed itemset $l'$ of size $k$ an entry $l'.frequent$ which is *true* if $l'$ was already determined to be NB-frequent, and a counter $l'.count$ to keep track of the number of NB-frequent $(k-1)$-subsets for which $l'$ was already accepted as a candidate.

1. $L = \{l \cup \{c\} | c \in C\}$
2. **foreach** candidate itemset $l' \in L$ **do begin**
3. **if** $l' \notin \mathcal{R}$ **then** add $l'$ with $l'.frequent = false$ and $l'.count = 0$ to $\mathcal{R}$
4. **if** $l'.frequent == true$ **then** delete $l'$ from $L$
5. **else begin**
6. $l'.count{+}{+}$
7. **if** $l'.count < \theta|l'|$ **then** delete $l'$ from $L$
8. **else** $l'.frequent = true$
9. **end**
10. **end**
11. **return** $L$

used in this paper in the plots in Fig. 4. In the left-hand side plots we see that by reducing $\pi$ the number of generated NB-frequent itemsets increases for all settings of $\theta$. For the most restrictive setting $\theta = 1$, pruning is maximal and the number of NB-frequent itemsets only increases at a very moderate rate with falling $\pi$. For $\theta = 0$, no pruning is conducted and the number of NB-frequent itemsets explodes already at relatively high values of $\pi$. At the intermediate setting of $\theta = 0.5$, the number of NB-frequent itemsets grows at a rate somewhere in between the two extreme settings. Although, for the extreme settings all three data sets react similarly, for $\theta = 0.5$ there is a clear difference visible between the real-world data sets and the artificial data set. While the magnitude of pruning for the real-world data sets is closer to $\theta = 0$, the magnitude for the artificial data set is closer to $\theta = 1$. Also, for the artificial data set we already find a relatively high number of NB-frequent itemsets at $\pi$ near to one (clearly visible for $\theta = 0$ and $\theta = 0.5$), a characteristic which the real-world data sets do not show. This characteristic is due to the way by which the used generator produces the data set from maximal potentially large itemsets (see Agrawal and Srikant (1994)).

As for most other mining algorithms, the number of generated itemsets has a direct influence on the execution time needed by the algorithm. To analyze the influence of the growth of the number of NB-frequent itemsets with falling values for parameter $\pi$, we recorded the CPU time[2] needed by the algorithm for the data sets in Fig. 4. The results for the setting $\theta = 0.5$ and the three data sets is presented in Table 8. As for other algorithms, execution time mainly depends on the search space size (given by the number of items) and the structure (or sparseness) of the data set. Compared to the other two data sets, WebView-1 has fewer items and is extremely sparse with very short transactions (on average only 2.5 items). Therefore, the algorithm needs to search through less itemsets and takes less time (between 0.55 and 6.98 seconds for values of $\pi$ between 0.999 and 0.7). Within each data set the execution time for different settings of the parameter $\pi$

[2]We used a machine with two Intel Xeon processors (2.4 GHz) running Linux (Debian Sarge). The algorithm was implemented in JAVA and compiled using the gnu ahead-of-time compiler gcj version 3.3.5. CPU time was recorded using the time command and we report the sum of user and system time.

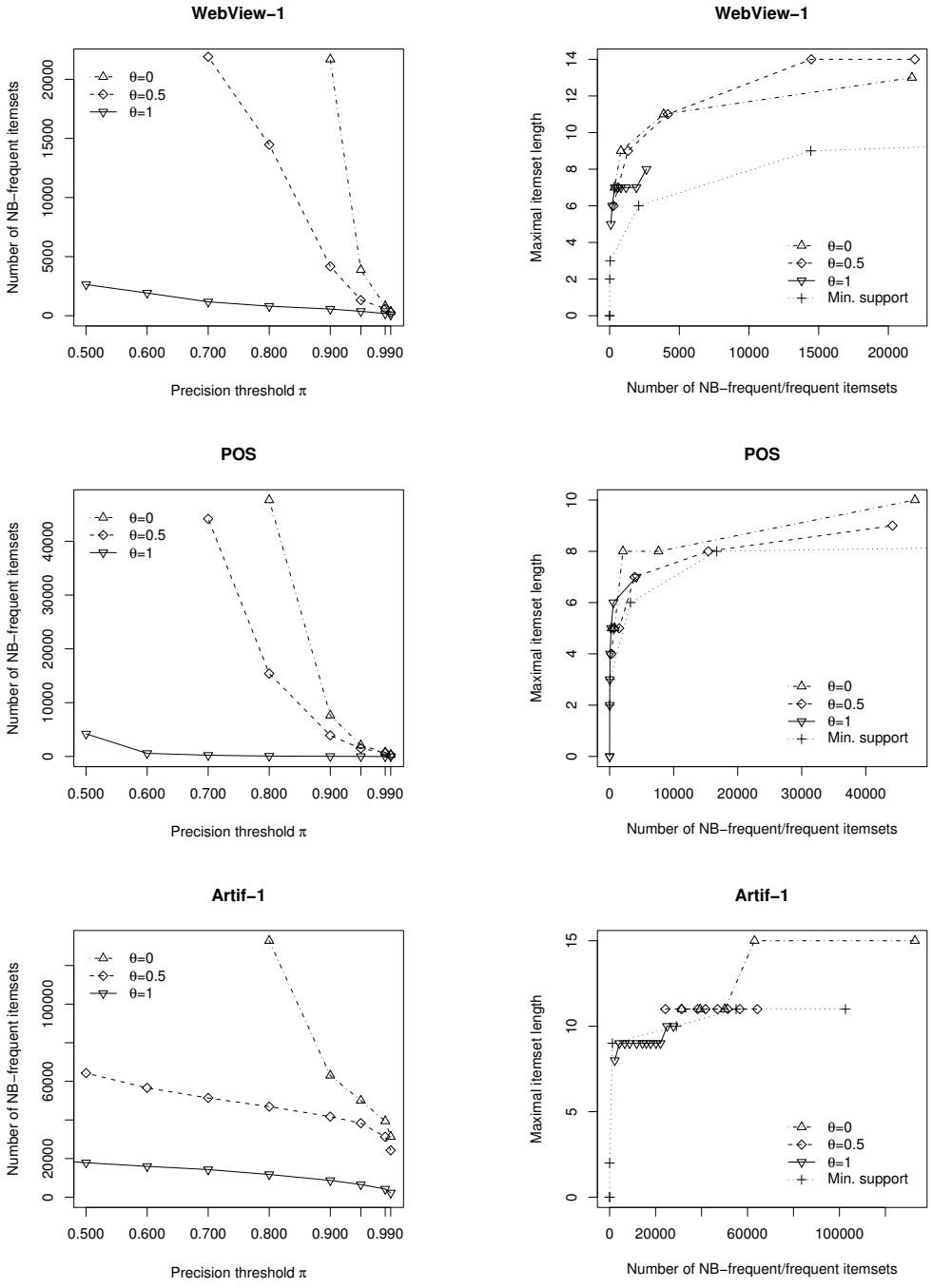



Figure 4: Comparison of the number of generated NB-frequent itemsets for different parameter settings.

Table 8: CPU-time in seconds to mine 20,000 transactions of the data sets using $\theta = 0.5$.

| $\pi$ | **WebView-1** | **POS** | **Artif-1** |
|---|---|---|---|
| 0.999 | 0.55 | 4.05 | 13.21 |
| 0.99 | 0.67 | 4.85 | 15.03 |
| 0.95 | 0.92 | 6.14 | 17.32 |
| 0.9 | 1.61 | 12.38 | 18.27 |
| 0.8 | 3.88 | 36.90 | 19.28 |
| 0.7 | 6.98 | 80.66 | 20.81 |

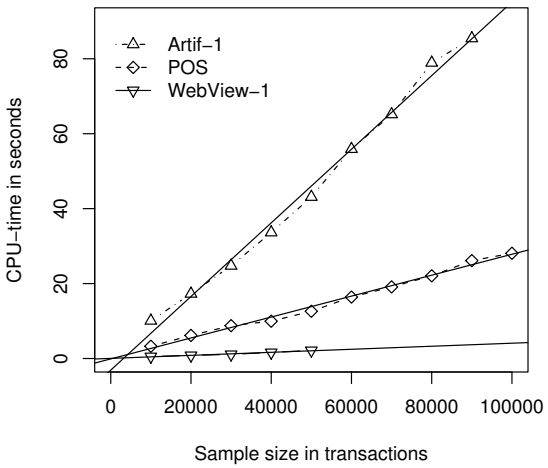



Figure 5: Relationship between execution time and data set size for the setting $\pi = 0.95$ and $\theta = 0.5$.

depends on how much of the search space needs to be traversed. Since the traversed search space and the number of generated NB-frequent itemsets is inversely related, the needed time grows close to linear with the number of found NB-frequent itemsets (compare the execution times with the left-hand side plots in Fig. 4). As for other algorithms, we can see from the pseudocode of the algorithm, that execution time is roughly linear in the number of transactions. This is supported by the experimental results for different size samples from the three data sets displayed in Fig. 5.

Next, we analyze the size of the accepted itemsets. For comparison we generated frequent itemsets using the implementations of Apriori and Eclat by Christian Borgelt[3]. We varied the minimum support threshold $\sigma$ between 0.1 and 0.0005. These settings were found after some experimentation to work best for the data sets. In the plots to the right in Fig. 4 we show the maximal itemset length by the number of accepted (NB-frequent or frequent) itemsets for the data sets and the settings used in the plot to the left. Naturally, the maximal length grows for all settings with the number of accepted itemsets which in turn grows with a decreasing precision threshold $\pi$ or minimum support $\sigma$. For the real-world data sets, NB-DFS tends to accept longer itemsets for the same number of accepted itemsets than minimum support. For the artificial data a clear difference is only visible for the setting $\theta = 0$.

The longer maximal itemset size for the model-based algorithm is caused by NB-Select's way of choosing an individual frequency constraint for all 1-extensions of an NB-frequent itemset. To analyze this behavior, we look at the minimum supports required by NB-Select for the data set

[3]Available at http://fuzzy.cs.uni-magdeburg.de/~borgelt/software.html

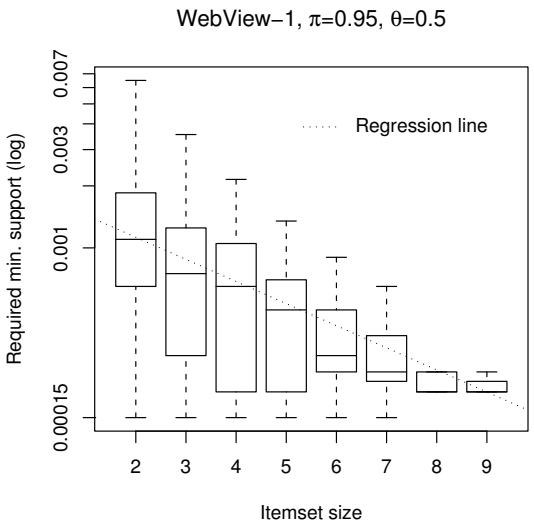



Figure 6: Boxplot of the minimum support required by NB-Select for the 1-extensions of NB-frequent itemsets of different size.

WebView-1 at $\pi = 0.95$ and $\theta = 0.5$. In Fig. 6 we use a box-and-whisker plot to represent the distributions of the minimum support thresholds required by NB-Select for different itemset sizes. The lines inside the boxes represent the median required minimum supports, the box spans from the lower to the upper quartile of the values, and the whiskers extend from the minimum to the maximum. The plot shows that the required support falls with itemset size.

Seno and Karypis (2001) already proposed to reduce the required support threshold with itemset size to improve the chances of finding longer maximal frequent itemsets without being buried in millions of shorter frequent itemsets. Instead of a fixed minimum support they suggested using a minimum support function which decreases with itemset size. Seno and Karypis (2001) used in their example a linear function together with an absolute minimum, however, the optimal choice of a support function and its parameters is still an open research question. In contrast to their approach, there is no need to specify such a function for the model-based frequency constraint since NB-Select automatically adjusts support for all 1-extensions of a NB-frequent itemset. In Fig. 6 we see that the average required minimum support falls roughly at a constant rate with itemset size (the dotted straight line in the plot represents the result of a linear regression on the logarithm of the required minimum supports). Reducing support with itemset size by a constant rate seems to be more intuitive than using a linear function.

## 5.2 Effectiveness of Pattern Discovery

After we studied the itemset generation behavior of the model-based algorithm and its ability to accept longer itemsets than minimum support, we need to evaluate if these additionally discovered itemsets represent non-spurious associations in the database. For the evaluation we need to know what true associations exist in the data and then compare how effective the algorithm is in discovering these itemsets. Since for most real-world data sets the underlying associations are unknown, we resort to artificial data sets, where the generation process is known and can be completely controlled.

To generate artificial data sets we use the popular generator developed by Agrawal and Srikant (1994). To evaluate the effectiveness of association discovery, we need to know all associations which were used to generate the data set. In the original version of the generator only the associations with the highest occurrence probability are reported. Therefore, we adapted the

code of the generator so that all used associations (called maximal potentially large itemsets) are reported. We generated two artificial data sets using this modified generator. Both data sets consist of $|\mathcal{D}| = 100,000$ transactions, the average transaction size is $|T| = 10$, the number of items is $N = 1,000$, and for the correlation and corruption levels we use the default values (0.5 for both).

The first data set, Artif-1, represents the standard data set T10I4D100K presented by Agrawal and Srikant (1994) and which is used for evaluation in many papers. For this data set $|L| = 2,000$ maximal potentially large itemsets with an average size of $|I| = 4$ are used.

For the second data set, Artif-2, we decrease the average association size to $|I| = 2$. This will produce more maximal potentially large itemsets of size one. These 1-itemsets are not useful associations since they do not provide information about dependencies between items. They can be considered noise in the generated database and, therefore, make finding longer associations more difficult. A side effect of reducing the average association size is that the chance of using longer maximal potentially large itemsets for the database generation is reduced. To work against this effect, we double their number to $|L| = 4,000$.

For the experiments, we use for both data sets the first $20,000$ transactions for mining associations. To analyze how the effectiveness is influenced by the data set size, we also report results for sizes $5,000$ and $80,000$ for Artif-2. For the model-based algorithm we estimated the parameters of the model from the data sets and then mined NB-frequent itemsets with the settings $0, 0.5$ and 1 for $\theta$. For each of the three settings for $\theta$, we varied the parameter $\pi$ between 0.999 and 0.1 (0.999, 0.99, 0.95, 0.9, 0.8 and in 0.1 steps down to 0.1). Because of combinatorial explosion discussed in the previous section, we only used $\pi \geq 0.5$ for $\theta = 0.5$ and $\pi \geq 0.8$ for $\theta = 0$.

For comparison with existing methods we mined frequent itemsets at minimum support levels between 0.1 and 0.0005 (0.01, 0.005, 0.004, 0.003, 0.002, 0.0015, 0.0013, 0.001, 0.0007, and 0.0005). And as a second benchmark we generated itemsets using all-confidence. We varied the threshold on all-confidence between 0.01 and 0.6 (0.6, 0.5, 0.4, 0.3, 0.2, 0.1, 0.05, 0.04, 0.03, 0.02, 0.01). The used minimum support levels and all-confidence thresholds were found after some experimentation to cover a wide area of the possible true positives/false positives combinations for the data sets.

To compare the ability to discover associations which were used to generate the artificial data sets, we counted the true positives (itemsets and their subsets discovered by the algorithm which were used in the data set generation process) and false positives (mined itemsets which were not used in the data set generation process). This information together with the total number of all positives in the database (all itemsets used to generate a data set) is used to calculate precision (the ratio of the number of true positives by the number of all instances classified as positives) and recall (the ratio of the number of true positives by the total number of positives in the data). Precision/recall plots, a common evaluation tool in information retrieval and machine learning, are then used to visually inspect the algorithms' effectiveness over their parameter spaces.

In Fig. 7, we inspect the effectiveness of the algorithm using the three settings for $\theta$. For comparison we add the precision/recall curves for minimum support and all-confidence. The top right corner of each precision/recall plot represents the optimal combination where all associations are discovered (recall = 1) and no false itemset is selected (precision = 1). Curves that are closer to the top right corner represent better retrieval effectiveness.

The precision/recall plots show that with $\theta = 1$ and $\pi \geq 0.5$ reachable recall is comparably low, typically smaller than 0.5, while precision is always high. On the data sets with 20,000 transactions it shows similar effectiveness as all-confidence. However, it outperforms all-confidence considerably on the small data set (Artif-2 with 5,000 transactions) while it is outperformed by all-confidence on the larger data set (Artif-2 with 80,000 transactions). This observation suggests that, if only little data is available, the additional knowledge of the structure of the data is more helpful.

With $\theta = 0$, where the generation is least strict, the algorithm reaches higher recall but precision deteriorates considerably with increased recall. The effectiveness is generally better than minimum support and all-confidence. Only for settings with very low values for $\pi$, precision degrades so strongly that its effectiveness is worse than minimum support and all-confidence. This effect can be seen in Fig. 7 for data set Artif-2 with 80,000 transactions.

The model-based algorithm with $\theta = 0.5$ performs overall the best with high recall while loosing

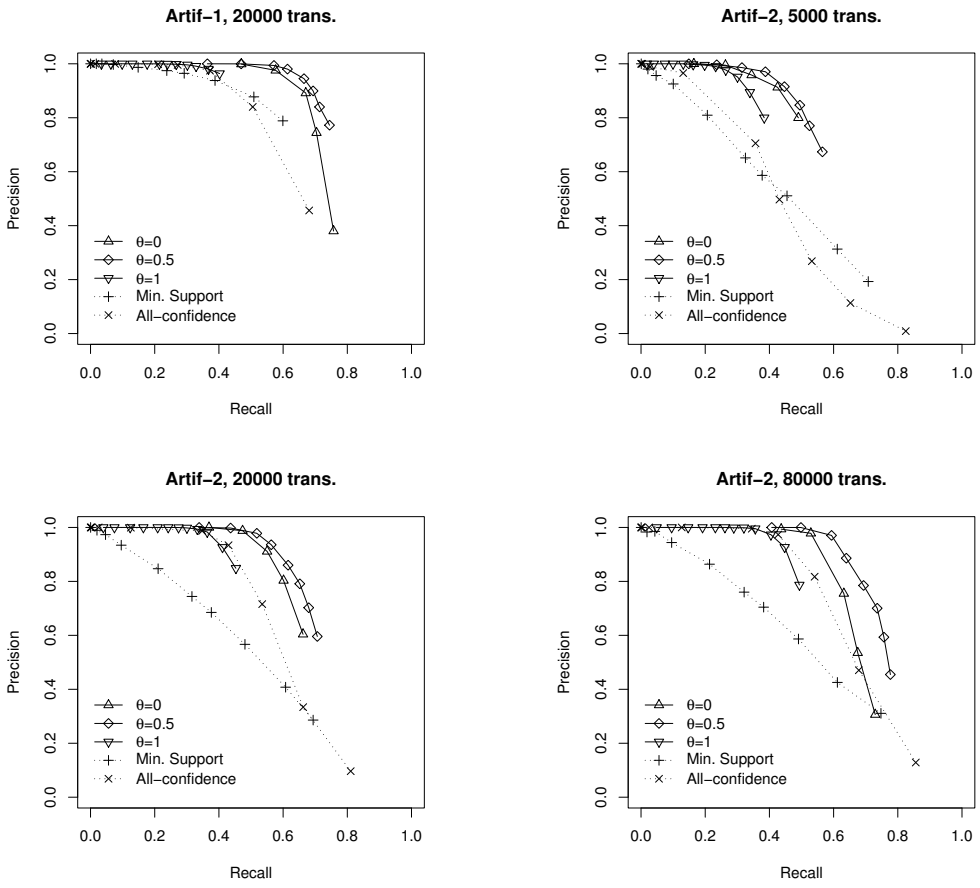



Figure 7: Comparison of the effectiveness of the model-based constraint with different settings for $\theta$.

Table 9: Relative differences of precision and recall between the results from data sets Artif-1 and Artif-2 (both with 20,000 transactions).

| | Precision | Recall |
|---|---|---|
| $\theta = 1$ | 15.94% | 1.54% |
| $\theta = 0.5$ | 6.86% | 8.32% |
| $\theta = 0$ | 16.88% | 14.09% |
| Min. support | 30.65% | 23.37% |
| All-confidence | 79.49% | 17.31% |

Table 10: Comparison of the set precision threshold $\pi$ and the actual precision of the mined associations for $\theta = 0.5$ on data set Artif-2 with 80,000 transactions.

| $\pi$ | precision |
|---|---|
| 0.999 | 1.0000000 |
| 0.990 | 0.9997855 |
| 0.950 | 0.9704649 |
| 0.900 | 0.8859766 |
| 0.800 | 0.7848500 |
| 0.700 | 0.7003764 |
| 0.600 | 0.5931635 |
| 0.500 | 0.4546763 |

less precision than $\theta = 0$. Its effectiveness clearly beats minimum support, all-confidence, and the model based algorithm with settings $\theta = 0$ and $\theta = 1$ on all data sets.

Comparing the two precision/recall plots for the data sets with 20,000 transactions in Fig. 7 shows that the results of the model-based constraint (especially for $\theta = 0.5$) dependent less on the structure and noise of the data set. To quantify this finding, we calculate the relative differences between the resulting precision and recall values for each parameter setting of each algorithm. In Table 9 we present the average of the relative differences per algorithm. While precision differs for support between the two data sets on average by about 30%, all-confidence exhibits an average difference of nearly 80%. Both values clearly indicate, that the optimal choice of the algorithms' parameters differs significantly for the two data sets. The model-based algorithm only differs by less than 20%, and with $\theta = 0.5$ the precision difference is only about 7%. This suggests that setting an average value for $\pi$ (e.g., 0.9) will produce reasonable results independently of the data set. The user only needs to resort to experimentation with different settings for the parameter, if she needs to optimize the results.

For an increasing data set size (see Artif-2 with 80,000 transactions in Fig. 7) and for the model-based algorithm at a set $\pi$, recall increases while at the same time precision decreases. This happens because with more available data NB-Select's predictions for precision get closer to the real values. In Table 10, we summarize the actual precision of the mined associations with $\theta = 0.5$ at different settings for the precision threshold. The close agreement between the columns indicates that, with enough available data, the set threshold on the predicted precision gets close to the actual precision of the set of mined associations. This is an important property of the model-based constraint, since it makes the precision parameter easier to understand and set for the person who applies data mining. While suitable thresholds on measures as support and all-confidence are normally found for each data set by experimentation, the precision threshold can be set with a needed minimal precision (or maximal acceptable error rate) for an application in mind.

A weakness of precision/recall plots and many other ways to measure accuracy is that they are only valid for comparison under the assumption of uniform misclassification cost, i.e., the error cost for false positives and false negatives are equal. A representation that does not depend on

uniform misclassification cost is the *Receiver Operator Characteristics graphs* (ROC graphs) used in machine learning to compare classifier accuracy (Provost and Fawcett, 1997). It is independent of class distribution (proportion of true positives to true negatives) and the distribution of misclassification costs. A ROC graph is a plot with the *false positive rate* on the x-axis and the *true positive rate* on the y-axis and represents the possible error trade-offs for each classifier. If a classifier can be parametrized, the points obtained using different parameters can be connected by a line called a *ROC curve.* If all points of one classifier are superior to the points of another classifier, the first classifier is said to dominates the latter one. This means that for all possible cost and class distributions, the first classifier can produce better results. We also examined ROC curves (omitted here due to space restrictions) for the data sets producing basically the same results as the precision/recall plots. The model-based frequency constraint with $\theta = 0.5$ clearly dominates all other settings as well as minimum support and all-confidence.

The results from artificial data sets presented here might not carry over 100% to real-world data sets. However, the difference between the effectiveness of the model-based constraint with $\theta = 0.5$ and minimum support or all-confidence is so big, that also on real-world data a significant improvement can be expected.

# 6 Conclusion

The contribution of this paper is that we presented a model-based alternative to using a single, user-specified minimum support threshold for mining associations in transaction data. We extended a simple and robust stochastic mixture model (the NB model) to develop a baseline model for incidence counts (co-occurrences of items) in the database. The model is easy to fit to data and explains co-occurrences counts between independent items. Together with a user-specified precision threshold, a local frequency constraint (support threshold) for all 1-extensions of an itemset can be found. The precision threshold represents the predicted error rate in the mined set of associations and, therefore, it is easy to specify by the user with the requirements of a specific application in mind.

Based on the developed model-based frequency constraint, we introduced the notion of NB-frequent itemsets and presented a prototypical mining algorithm to find all NB-frequent itemsets in a database. Although the definition of NB-frequency, which is based on local frequency constraints, does not provide the important downward closure property of support, we showed how the search space can be adequately reduced to make efficient mining possible.

Experiments showed that the model-based frequency constraint automatically reduces the average needed frequency (support) with growing itemset size. Compared with minimum support it tends to be more selective for shorter itemsets while still accepting longer itemsets with lower support. This property reduces the problem of being buried in a great number of short itemsets when using a relatively low threshold in order to also find longer itemsets.

Further experiments on artificial data sets indicate that the model-based constraint is more effective in finding non-spurious associations. The largest improvements were found for noisy data sets or when only a relatively small database is available. These experiments also show that the precision parameter of the model-based algorithm depends less than support or any-confidence on the data set. This is a huge advantage and reduces the need for time-consuming experimentation with different parameter settings for each new data set.

Finally, it has to be noted that the model-based constraint developed in this paper can only be used for databases which are generated by a process similar to the developed baseline model. The developed baseline is a robust and reasonable model for most transaction data (e.g., point-of-sale data). For other types of data, different baseline models can be developed and can then be incorporated in mining algorithms following the outline of this paper.

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